Douglas E Spearot

List of Publications by Year
in descending order

86	2,538	218381	214527
papers	citations	26 h-index	47 g-index

87	87	87	2228
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Tensile strength of âŒ©100âŒª and âŒ©110âŒª tilt bicrystal copper interfaces. Acta Materialia, 2007, 55, 705-714.	3.8	217
2	Nucleation of dislocations from [001] bicrystal interfaces in aluminum. Acta Materialia, 2005, 53, 3579-3589.	3.8	194
3	Dislocation nucleation from bicrystal interfaces with dissociated structure. International Journal of Plasticity, 2007, 23, 143-160.	4.1	153
4	Two-dimensional MoS₂ under ion irradiation: from controlled defect production to electronic structure engineering. 2D Materials, 2017, 4, 025078.	2.0	146
5	Dislocation nucleation from bicrystal interfaces and grain boundary ledges: Relationship to nanocrystalline deformation. Journal of the Mechanics and Physics of Solids, 2007, 55, 2300-2327.	2.3	121
6	Atomistic simulations of homogeneous dislocation nucleation in single crystal copper. Modelling and Simulation in Materials Science and Engineering, 2007, 15, 693-709.	0.8	114
7	Insights on slip transmission at grain boundaries from atomistic simulations. Current Opinion in Solid State and Materials Science, 2014, 18, 188-195.	5.6	102
8	Non-local separation constitutive laws for interfaces and their relation to nanoscale simulations. Mechanics of Materials, 2004, 36, 825-847.	1.7	88
9	Fracture mechanics of monolayer molybdenum disulfide. Nanotechnology, 2015, 26, 175703.	1.3	70
10	Effect of point and grain boundary defects on the mechanical behavior of monolayer MoS2 under tension via atomistic simulations. Journal of Applied Physics, 2014, 116, 013508.	1.1	64
11	Influence of Grain Boundary Structure on Dislocation Nucleation in FCC Metals. Dislocations in Solids, 2008, 14, 43-139.	1.6	57
12	Simultaneous twinning and microband formation under dynamic compression in a high entropy alloy with a complex energetic landscape. Acta Materialia, 2020, 200, 1-11.	3.8	55
13	Visco-hyperelastic constitutive modeling of strain rate sensitive soft materials. Journal of the Mechanics and Physics of Solids, 2020, 135, 103777.	2.3	53
14	Atomistic Modeling of Grain Boundaries and Dislocation Processes in Metallic Polycrystalline Materials. Journal of Engineering Materials and Technology, Transactions of the ASME, 2009, 131, .	0.8	40
15	A Computational Algorithm to Produce Virtual X-ray and Electron Diffraction Patterns from Atomistic Simulations. Jom, 2014, 66, 408-416.	0.9	40
16	Phase transformation in monolayer molybdenum disulphide (MoS2) under tension predicted by molecular dynamics simulations. Scripta Materialia, 2014, 76, 41-44.	2.6	36
17	A molecular dynamics study of dislocation density generation and plastic relaxation during shock of single crystal Cu. Journal of Applied Physics, 2016, 120, .	1.1	36
18	Mobility of dislocations in Aluminum: Faceting and asymmetry during nanoscale dislocation shear loop expansion. Acta Materialia, 2019, 168, 426-435.	3.8	36

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19	Tractionâ€“separation relationships for hydrogen induced grain boundary embrittlement in nickel via molecular dynamics simulations. Materials Science & Engineering A: Structural Materials: Properties, Microstructure and Processing, 2016, 650, 354-364.	2.6	35
20	Evolution of the E structural unit during uniaxial and constrained tensile deformation. Mechanics Research Communications, 2008, 35, 81-88.	1.0	34
21	Molecular dynamics simulation of the shock response of materials: A tutorial. Journal of Applied Physics, 2022, 131, .	1.1	32
22	Thermodynamics-based stability criteria for constitutive equations of isotropic hyperelastic solids. Journal of the Mechanics and Physics of Solids, 2019, 124, 115-142.	2.3	30
23	Hyperelastic constitutive modeling of hydrogels based on primary deformation modes and validation under 3D stress states. International Journal of Engineering Science, 2020, 154, 103314.	2.7	30
24	Molecular Dynamics Simulation of Nanoconfinement Induced Organization of n-Decane. Langmuir, 2009, 25, 7553-7560.	1.6	29
25	Microstructural stability of copper with antimony dopants at grain boundaries: experiments and molecular dynamics simulations. Journal of Materials Science, 2010, 45, 6707-6718.	1.7	29
26	Plastic deformation of nanocrystalline copper-antimony alloys. Journal of Materials Research, 2010, 25, 411-421.	1.2	29
27	On the elastic tensile deformation of ã€˜100ã€‰ bicrystal interfaces in copper. Computational Materials Science, 2008, 42, 57-67.	1.4	28
28	A molecular dynamics study of the role of grain size and orientation on compression of nanocrystalline Cu during shock. Computational Materials Science, 2015, 108, 226-232.	1.4	25
29	Shock compression of Cu x Zr100â^'x metallic glasses from molecular dynamics simulations. Journal of Materials Science, 2018, 53, 5719-5732.	1.7	23
30	A primer on selecting grain boundary sets for comparison of interfacial fracture properties in molecular dynamics simulations. Scientific Reports, 2017, 7, 8332.	1.6	22
31	Mobility of dislocations in aluminum: The role of non-Schmid stress state. Acta Materialia, 2020, 185, 420-432.	3.8	22
32	Mobility of dislocations in FeNiCrCoCu high entropy alloys. Modelling and Simulation in Materials Science and Engineering, 2021, 29, 085017.	0.8	22
33	Effect of deformation path sequence on the behavior of nanoscale copper bicrystal interfaces. Journal of Engineering Materials and Technology, Transactions of the ASME, 2005, 127, 374-382.	0.8	19
34	Heterogeneous dislocation nucleation in single crystal copperâ€“antimony solid-solution alloys. Modelling and Simulation in Materials Science and Engineering, 2009, 17, 055001.	0.8	19
35	Atomic-level deformation of Cu_xZr₁₀₀₋_x metallic glasses under shock loading. Journal of Applied Physics, 2018, 123, 215101.	1.1	19
36	Spectrum of embrittling potencies and relation to properties of symmetric-tilt grain boundaries. Acta Materialia, 2021, 205, 116527.	3.8	19

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37	Phase-field simulations of microstructure evolution during physical vapor deposition of single-phase thin films. Computational Materials Science, 2017, 131, 170-177.	1.4	18
38	Nanoscale dislocation shear loops at static equilibrium and finite temperature. Modelling and Simulation in Materials Science and Engineering, 2017, 25, 085014.	0.8	18
39	Effect of water concentration on the shock response of polyethylene glycol diacrylate (PEGDA) hydrogels: A molecular dynamics study. Journal of the Mechanical Behavior of Biomedical Materials, 2019, 90, 30-39.	1.5	17
40	Molecular dynamics simulation of O₂diffusion in polydimethylsiloxane (PDMS) and end-linked PDMS networks. Molecular Simulation, 2014, 40, 976-986.	0.9	16
41	Void collapse and subsequent spallation in Cu50Zr50 metallic glass under shock loading by molecular dynamics simulations. Journal of Applied Physics, 2019, 125, .	1.1	16
42	Integrating in situ TEM experiments and atomistic simulations for defect mechanics. Current Opinion in Solid State and Materials Science, 2019, 23, 117-128.	5.6	16
43	Structure and kinetics of three-dimensional defects on the <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si1.svg"><mml:mrow><mml:mo>{</mml:mo><mml:mrow><mml:mn>10</mml:mn><mml:mover accent="true"><mml:mn>1</mml:mn><mml:mo>Â¯</mml:mo></mml:mover><mml:mn>2</mml:mn></mml:mrow><mml:mo>}</mml:mo></mml:m twin boundary in magnesium: Atomistic and phase-field simulations. Mechanics of Materials, 2020, 143, 103314.	1.7	16
44	Influence of vacancy defect concentration on the combustion of reactive Ni/Al nanolaminates. Journal of Applied Physics, 2018, 124, .	1.1	15
45	Microstructure stability of nanocrystalline materials using dopants. Molecular Simulation, 2008, 34, 35-40.	0.9	14
46	Molecular Dynamics Simulations of Dislocation Activity in Single-Crystal and Nanocrystalline Copper Doped with Antimony. Metallurgical and Materials Transactions A: Physical Metallurgy and Materials Science, 2010, 41, 854-860.	1.1	14
47	The effect of synthetic driving force on the atomic mechanisms associated with grain boundary motion below the interface roughening temperature. Computational Materials Science, 2014, 86, 38-42.	1.4	14
48	Phase-field models for simulating physical vapor deposition and grain evolution of isotropic single-phase polycrystalline thin films. Computational Materials Science, 2016, 123, 111-120.	1.4	14
49	Role of grain boundary structure on diffusion and dissolution during Ni/Al nanolaminate combustion. Journal of Applied Physics, 2020, 127, .	1.1	14
50	Effect of the initial temperature on the shock response of Cu50Zr50 bulk metallic glass by molecular dynamics simulation. Journal of Applied Physics, 2021, 129, .	1.1	14
51	Molecular dynamics simulation of diffusion of small atmospheric penetratesin polydimethylsiloxane. Molecular Simulation, 2011, 37, 115-122.	0.9	12
52	Pressure Dependence of the Peierls Stress in Aluminum. Jom, 2018, 70, 1094-1099.	0.9	12
53	Transient-State Rheological Behavior of Poly(ethylene glycol) Diacrylate Hydrogels at High Shear Strain Rates. Macromolecules, 2019, 52, 5860-5871.	2.2	12
54	Fracture mechanics of multi-layer molybdenum disulfide. Engineering Fracture Mechanics, 2019, 212, 1-12.	2.0	12

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55	Validated tensile characterization of the strain rate dependence in soft materials. International Journal of Impact Engineering, 2021, 156, 103949.	2.4	12
56	Shear-driven motion of Mg <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mo>{</mml:mo><mml:mrow><mml:mn>10</mml:mn><mml accent="true"><mml:mn>1</mml:mn><mml:mo>Â¯</mml:mo></mml:mover><mml:mn>2</mml:mn></mml:mrow><mml:mo> twin boundaries via disconnection terrace nucleation, growth, and coalescence. Physical Review Materials, 2019, 3, .	2.9	12
57	Interatomic potential for copperâ€“antimony in dilute solidâ€“solution alloys and application to single crystal dislocation nucleation. Computational Materials Science, 2009, 44, 1258-1264.	1.4	11
58	Melting of Ni and Fe Nanoparticles: A Molecular Dynamics Study with Application to Carbon Nanotube Synthesis. Journal of Nanoscience and Nanotechnology, 2010, 10, 5587-5593.	0.9	11
59	Molecular Dynamics Simulations of Diffusion of O2 and N2 Penetrants in Polydimethylsiloxane-Based Nanocomposites. Journal of Engineering Materials and Technology, Transactions of the ASME, 2012, 134, .	0.8	11
60	Atomistic simulation and virtual diffraction characterization of homophase and heterophase alumina interfaces. Acta Materialia, 2015, 82, 403-413.	3.8	11
61	Mechanical properties of stabilized nanocrystalline FCC metals. Journal of Applied Physics, 2019, 126, .	1.1	11
62	Atomistic simulation and virtual diffraction characterization of stable and metastable alumina surfaces. Acta Materialia, 2014, 78, 354-368.	3.8	10
63	Grain size effects on Ni/Al nanolaminate combustion. Journal of Materials Research, 2019, 34, 2229-2238.	1.2	9
64	Mechanical behavior of coreâ€“shell nanostructures. Journal of Materials Science, 2020, 55, 4303-4310.	1.7	9
65	Disclination-dislocation based model for grain boundary stress field evolution due to slip transmission history and influence on subsequent dislocation transmission. Journal of the Mechanics and Physics of Solids, 2022, 165, 104920.	2.3	9
66	Effect of Loop Defects on the High Strain Rate Behavior of PEGDA Hydrogels: A Molecular Dynamics Study. Journal of Physical Chemistry B, 2020, 124, 2029-2039.	1.2	8
67	Behavior of dopant-modified interfaces in metallic nanocrystalline materials. Jom, 2010, 62, 70-74.	0.9	7
68	Virtual diffraction analysis of dislocations and dislocation networks in discrete dislocation dynamics simulations. Computational Materials Science, 2020, 174, 109473.	1.4	7
69	Role of equilibrium and non-equilibrium grain boundary stress fields on dislocation transmission. Journal of Materials Research, 2021, 36, 2687-2704.	1.2	7
70	Bridging atomistic simulations and experiments via virtual diffraction: understanding homophase grain boundary and heterophase interface structures. Journal of Materials Science, 2016, 51, 1251-1260.	1.7	6
71	Simulation of kinematic Kikuchi diffraction patterns from atomistic structures. MethodsX, 2018, 5, 1187-1203.	0.7	6
72	An embedded-atom method potential parameterized for sulfur-induced embrittlement of nickel. Modelling and Simulation in Materials Science and Engineering, 2019, 27, 085016.	0.8	6

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73	Physical vapor deposition of multiphase materials with phase nucleation via a coupled phase-field approach. Computational Materials Science, 2018, 143, 71-79.	1.4	5
74	Zr segregation in Niâ€“Zr alloy: implication on deformation mechanism during shear loading and bending creep. Journal of Materials Science, 2020, 55, 6172-6186.	1.7	5
75	Performance Improvement and Workflow Development of Virtual Diffraction Calculations. , 2014, , .		4
76	On shockwave propagation and attenuation in poly(ethylene glycol) diacrylate hydrogels. Journal of the Mechanical Behavior of Biomedical Materials, 2021, 118, 104423.	1.5	3
77	Atomistic Simulation Techniques to Model Hydrogen Segregation and Hydrogen Embrittlement in Metallic Materials. , 2018, , 1-34.		2
78	Molecular Dynamics Simulations of Dislocation Nucleation From Bicrystal Interfaces in FCC Metals. , 2005, , 505.		1
79	Experimental Characterization of DNA/CNT Hybrid Structures with Atomic Force Microscope. , 2008, , .		1
80	Algorithm Development in Computational Materials Science. Jom, 2014, 66, 397-398.	0.9	1
81	Role of grain boundaries and substrate in plastic deformation of coreâ€“shell nanostructures. Journal of Materials Science, 2020, 55, 16990-16999.	1.7	1
82	Nano-Particle Polymer Composite MEMS corrosion. , 2011, , .		0
83	Foreword: Modeling, Simulation, and Theory of Nanomechanical Materials Behavior. Metallurgical and Materials Transactions A: Physical Metallurgy and Materials Science, 2011, 42, 3867-3867.	1.1	0
84	Swell-based in situ oxide removal methods for PDMS-copper particle composite corrosion sensing elements. Proceedings of SPIE, 2012, , .	0.8	0
85	Atomistic Simulation Techniques to Model Hydrogen Segregation and Hydrogen Embrittlement in Metallic Materials. , 2019, , 357-390.		0
86	Data-driven analysis of neutron diffraction line profiles: application to plastically deformed Ta. Scientific Reports, 2022, 12, 5628.	1.6	0